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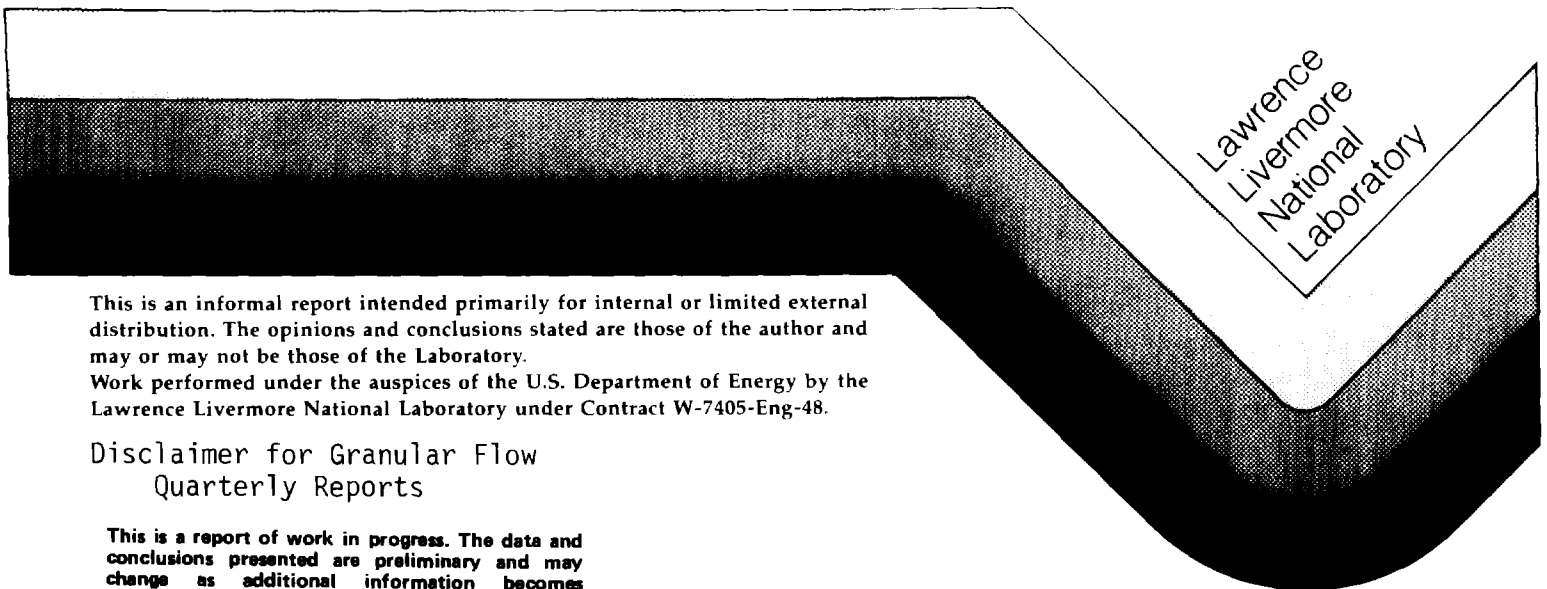
LAWRENCE LIVERMORE NATIONAL LABORATORY
GRANULAR FLOW PROJECT - QUARTERLY REPORT

April - June 1985

Edited by
O.R. Walton

For
U.S. Department of Energy
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April - June 1985

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The major effort of LLNL's Granular Flow Project during FY85 is the development and application of new discrete particle computer models for simulating the flow behavior of granular solids and determining their rheologic behavior. During the first two quarters of FY85 we developed and tested some of the fundamental building blocks of our new discrete models including new interparticulate force models for frictional, inelastic contacts between disks and spheres and a two-dimensional steady-state shearing model with periodic boundaries utilizing these new interaction models. Descriptions of the interparticulate force models, the steady shearing model and a preliminary two-dimensional shearing parameter study have already been reported^{1,2}.

The goals of LLNL's granular flow project include the development of small-cell discrete particle computer models for determining rheologic properties of granular solids and also larger models capable of direct simulation of the motion of thousands of particles through various geometries for direct application in engineering design calculations. During the current reporting period we have continued to work on various building blocks for a full three-dimensional shearing-cell model, and have also put considerable effort into getting a fully unified model running and producing results. Our "test-bed" model is a two-dimensional steady-state shearing-cell model with periodic boundaries, incorporating all of the building blocks developed to date. This model was selected as our first fully unified model because it utilized everything from uniform shearing with periodic boundaries to new

diagnostic averaging algorithms. Also, almost all of the development needed for this two-dimensional model is directly transferable to the full three-dimensional model under development. Specifically, during this reporting period we have: 1) determined an algorithm for incrementally slipping two-dimensional surface friction (acting between three-dimensional objects), 2) added features to the two-dimensional steady-state shearing model, such as internal averaging zones, real boundaries and velocity distribution calculations, 3) detected and corrected minor errors in the periodic-boundary shearing model, 4) conducted a parameter study on the effects of inelasticity and interparticulate friction on effective viscosity, granular-temperature and stresses in shearing assemblies of two-dimensional disks, and 5) reported the results of our research at technical meetings and journals. We report below the details of these activities.

2-D Analog to 1-D Incrementally Slipping Friction Model

When two bodies are in sliding contact the contact region deformation includes small (elastic, recoverable) shear and normal-direction strains, proportional in magnitude to the total tangential-friction and normal-direction forces acting over the contact area. Mathematical models of inter-particulate contacts often approximate the effects of these small deformations in (the contact region of) the particles by using a contact element that exhibits both shear and normal direction strains of finite magnitude. Our partially-latching-spring normal force and incrementally-slipping-friction model represents just such a contact element acting between essentially rigid particles. The tangential friction model associates a shear displacement, s , with the total tangential force, T , such that

$$T = -K_T s$$

where K_T is the effective tangential stiffness, which could be non-linear (as in our incrementally-slipping model). The tangential friction force, T , is also limited by the normal force, N , and the friction coefficient, μ , such that,

$$|T| \leq \mu N \quad .$$

In frictional contacts restricted to motion in one-dimension (i.e., between two-dimensional objects), any sliding is always in either the direction of increasing or decreasing the current recoverable shear strain. In two-dimensional contacts (i.e., between three-dimensional objects) the direction of the recoverable shear strain is usually aligned with the current direction of sliding; however, this alignment does not necessarily occur instantaneously when the direction of sliding changes. The usual rule for two-dimensional frictional contacts, that "when tangential motion occurs the friction force acts in the same direction as the relative velocity but in the opposite sense³" is valid for continuous sliding motion with very gradual changes in the slip direction; however, during rapid changes in the direction of relative slip (due to applied loads) the direction of true friction force acting between two bodies may lag slightly behind the change in the direction of the current relative slip velocity. We have developed a straight forward two-dimensional analogue to our previously reported one-dimensional incrementally-slipping friction model that combines the displacement-dependent hysteresis of our previous model with a realistic lag in change of direction of the recoverable-shear-strain vector during rapid changes in the direction of sliding. This model incrementally applies any change in relative position of a sliding contact in two steps: the first step determines the effect of any change in relative position parallel to the current recoverable-shear-strain vector; the second step determines the effect of motion perpendicular to the current recoverable-shear-strain vector. The lag

time for the calculated friction force direction change depends on the magnitude of the recoverable elastic shear strain which, in turn, depends on the magnitude of the normal force, N , and the tangential stiffness, K_T . We are currently programming this new model into a small two-particle collision code in order to test the sensitivity of collision trajectories to various choices of shear and normal stiffness.

Two-Dimensional Steady State Shearing Cell Model:

Improvements, Corrections and Calculations

Several modifications have been made to our steady-state-shearing, periodic-boundary model. Internal averaging zones have been added. Within each zone the program now calculates cumulative time averages of each stress tensor component, the mean and deviatoric particle velocities, the effective strain rate, the solids fraction in the zone, the potential and translational kinetic energy density, and the mean particle spin and other quantities. Many of these quantities scale with the mass in each zone. For simplicity, we assume that any particle spanning a zone boundary has its mass, and all mass related quantities, split between the two zones according to the fraction of the particle diameter (perpendicular to the zone boundary) that lies in each zone. This simplified approach (as opposed to calculating the fraction of the circular area that is in each zone) does not cause significant inaccuracies because the cumulative time averages are over a large number of positions for each particle and any slight inaccuracy in one instantaneous "snapshot" is lost in the statistics of the long-time averages. Figure 1 is a histogram plot of the cumulative time averages of the x-direction particle velocities in each of five zones in a steady state shearing calculation at a solids packing fraction of 0.60. The uniform variation of velocity across the primary cell seen in this figure results from the motion of the periodic image cells.

Figure 2 shows the distribution of rotational kinetic energy in the same calculation. These figures demonstrate that the steady state shearing model is producing the desired uniform shearing field with velocities and rotations nearly uniformly distributed across the calculational cell.

The inclusion of five internal zones in our nominal 30-particle system added roughly one third to the computer time required for a typical calculation on the CDC7600 computer. The added cost was soon justified when the improved diagnostics provided enough detail to detect a previously unnoticed error in the tangential friction force calculation affecting only those particles that were interacting with periodic images of particles from cells above or below the primary cell (this affected the tangential friction force only in the top and/or bottom zones and not the others). Correcting the error had a minor effect (i.e., less than 10%) on most calculated quantities reported in our last quarterly; however, it did have a significant effect on shearing behavior at high solids fractions and on the mean rotational velocities in all calculations. The (incorrect) order of magnitude decrease in stresses we reported² occurring at solids fractions between 0.725 and 0.750 now becomes a much more orderly transition from fluid-like behavior (with nearly uniform shearing) to a solid-like behavior (with a single rolling or shearing layer). The transition occurs at a solids fraction between 0.775 and 0.800. A decrease in stress of only about a factor of two is now calculated in going from the fluid-like behavior to the single shearing layer.

The data storage structure of the model was also modified to incorporate near-neighbor arrays and linked-list logic to more efficiently utilize both the memory and cpu of the computer. Using the new memory structure, any increase in the number of particles being calculated results in an almost

linear increase in the total amount of computer time required for a calculation. This is a significant improvement in efficiency over the old structure that had a second power dependence of computer time with number of particles calculated. With the new linked-list data structure up to approximately 400 particles can be calculated without needing to use the large-core memory on the CDC7600 computer and up to a few thousand could be calculated on that same computer if the near-neighbor array storage were moved to large-core memory. The new (near-neighbor) model reduces the computer time for a typical 30-particle problem by about 30% to 50%. The net result of both the improved efficiency and the increased number of diagnostic calculations is almost no net change in the total running time for a typical 30-particle problem which may take anywhere from 6 to 30 minutes of CDC7600 cpu time.

Another significant modification to our steady state shearing model was the removal of the artificial shearing force that had previously been used to aid in distributing the shear across the calculational cell. We found that inclusion of such an artificial force prevented the expected increase in mean deviatoric velocity as the solids packing fraction is decreased. The straight line trajectories between collisions in the present model produce significant increases in the mean deviatoric velocity of particles (in steady shearing) as the solids fraction is decreased. This modification had only a small effect on the stresses calculated at solids concentrations above $\nu = 0.60$; however, it did significantly change the calculated kinetic contribution to the stress tensor at low solids concentrations.

Figure 3 shows the total pressure and the kinetic and potential contributions to that total as calculated by the corrected model. The values shown on this figure are in agreement with predicted behavior for three-

dimensional granular materials in steady shear⁴ and with rigid body calculations of two-dimensional shear using particles with a nearly infinite friction coefficient⁵. We have also made other comparisons with smooth and rough two-dimensional rigid body calculations, three-dimensional experimental measurements and theoretical predictions and have every reason to believe that the results we are now calculating represent "real" behavior for assemblies of inelastic, frictional disks.

Other improvements to the model during this reporting period include adding the option of selecting real boundaries (instead of periodic ones) on the top and bottom boundaries of the primary calculational cell. We also added the option to include gravity, acting in any direction, in any real boundary calculation. These two changes will allow us to directly simulate vertical channel flow, incline plane flow and rectilinear shear flow between moving particle layers. University researchers at Clarkson⁶ and UCLA⁷ are currently working on experiments involving two-dimensional flows. As soon as we obtain detailed information on the mechanical and frictional properties of the particles to be used in those studies we will be able to make simulation calculations that can be compared directly with the planned experimental measurements.

We also added the capability to plot the cumulative time average of the particle velocity distribution in the entire calculational cell. Figure 4 shows a velocity distribution plot for a calculation at a solids fraction of 0.10 with highly dissipative interactions (i.e., $e = 0.6$, $\mu = 0.5$). The resulting velocity distribution is anisotropic with much wider spread in the x-direction than in the y-direction. The x-component of the pressure, p_{xx} , also exceeded the y-component, p_{yy} , by a significant factor in this calculation. At higher solids concentrations and with less dissipative interactions both the velocity and pressure became much more symmetric.

A set of calculations examining the effects of inelasticity and friction on the viscosity, granular-temperature and stresses in shearing assemblies of disks was completed using the periodic boundary model. Most of the calculated results were in agreement with expectations; however, we did calculate an increase in two-dimensional collisional contributions to the shear stresses when frictional effects (i.e., particle rotations) were included. This is in contradiction with the approximate three-dimensional theory of Lun et al.⁴ which predicts a decrease in collisional shear stresses with the inclusion of friction. A paper on this study has been submitted for publication in the Journal of Rheology.

Visitors (April - June 1985)

- Gisle Enstad - from Chs. Michelson Lab., Fantoft, Norway, May 2, 1985,
to discuss laboratory measurements of granular shear strengths,
and multi-layer chute flow tests at LLNL.
- Thomas Drake - from Earth & Space Sciences Dept., UCLA, April 5, 1985,
to discuss 2-D chute flow experiments and possible
collaborative work with LLNL.

Publications and Presentations (April - June 1985)

- O. R. Walton, "Computer simulation of Granular Flow", LLNL Report No. UCID-20411 (reprint from UCRL-52000-84-5), presented at International Fine Particle Research Institute's Annual Mtg., Chicago, Ill., 10-13 June 1985
- O.R. Walton and R.L. Braun, "Viscosity, Granular-Temperature and Stress Calculations For Shearing Assemblies of Inelastic, Frictional Disks", presented at 56th Annual Mtg. Soc. of Rheology, Blacksburg, VA, 24-27 February 1985 and submitted to Journal of Rheology, (LLNL Report No. UCRL-91756, June 25, 1985)

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1. Granular Flow Project Quarterly Report, Oct.-Dec. 1984, O. R. Walton, ed., LLNL Report UCID 20297-84-4.
2. Granular Flow Project Quarterly Report, Jan.-March 1985, O. R. Walton, ed., LLNL Report UCID 20297-85-1.
3. J. J. Oden and J. A. C. Martins, "Models and Computational Methods for Dynamic Friction Phenomena", proceedings, FENOMECH III, Stuttgart, W. Germany, Computer Methods in Appl. Mech. and Engng., North Holland, Amsterdam, 1984.
4. C. K. K. Lun, S. B. Savage, D. J. Jeffrey, and N. Chenpurniy, "Kinetic Theories for Granular Flow: Inelastic Particles in Couette Flow and Slightly Inelastic Particles in a General Flow Field", J. Fluid Mech. Vol. 140, 1984, pp. 223-256.
5. C. S. Campbell and A. Gong, "The Stress Tensor in a Two-Dimensional Granular Shear Flow", J. Fluid Mech. (in press).
6. H. Shen and N. Ackerman (private communication, 1985) Clarkson University, Potsdam, N.Y., (performing experiments with disks on a horizontal and/or slightly tilted air-table with moving and fixed boundaries).
7. T. G. Drake and R. L. Shreve, "High-speed Motion Pictures of Steady Parallel Two-Dimensional Inertial Flows of Granular Materials", presented at 56th Soc. of Rheology Mtg. 25-27 Feb. 1985, Blacksburg, VA. (2-D incline chute flow tests with polystyrene beads between parallel glass plates).

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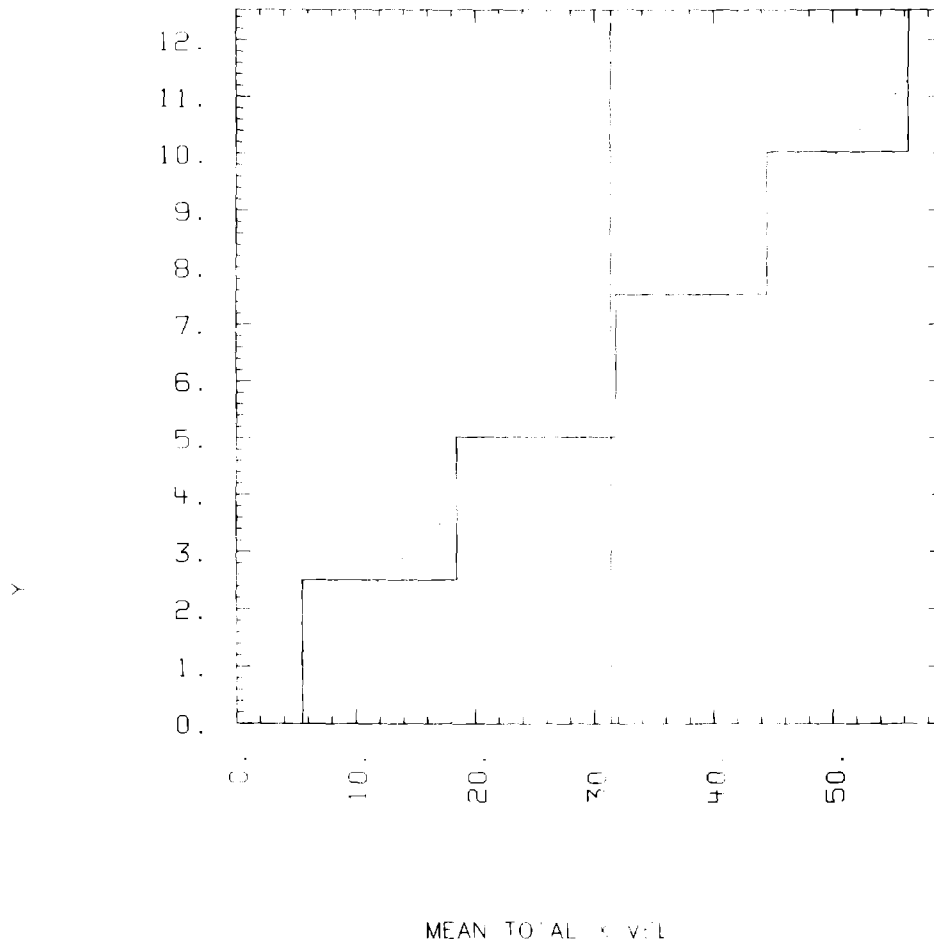


Fig. 1. Vertical distribution of mean x-direction particle velocities in a steady-state shearing calculation with five vertical averaging zones.

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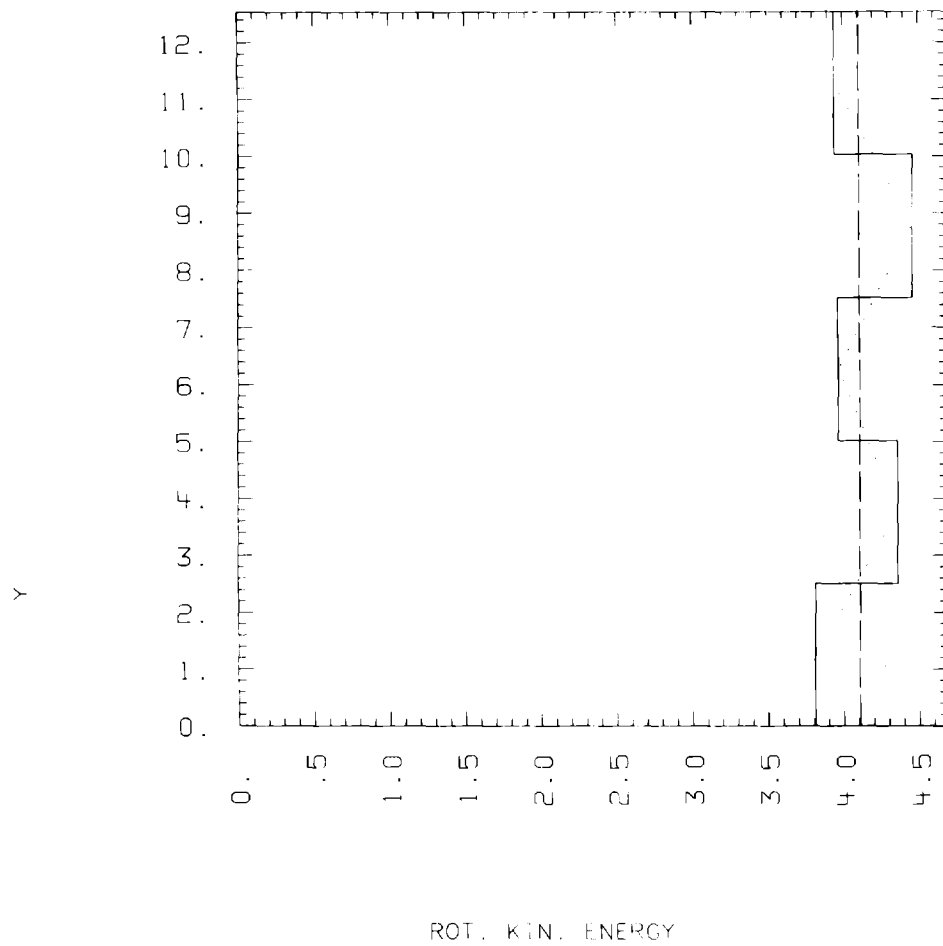


Fig. 2. Vertical distribution of mean rotational kinetic energy density in a steady state shearing calculation with five vertical zones ($e = 0.8$, $\mu = 0.5$, $\nu = 0.6$)

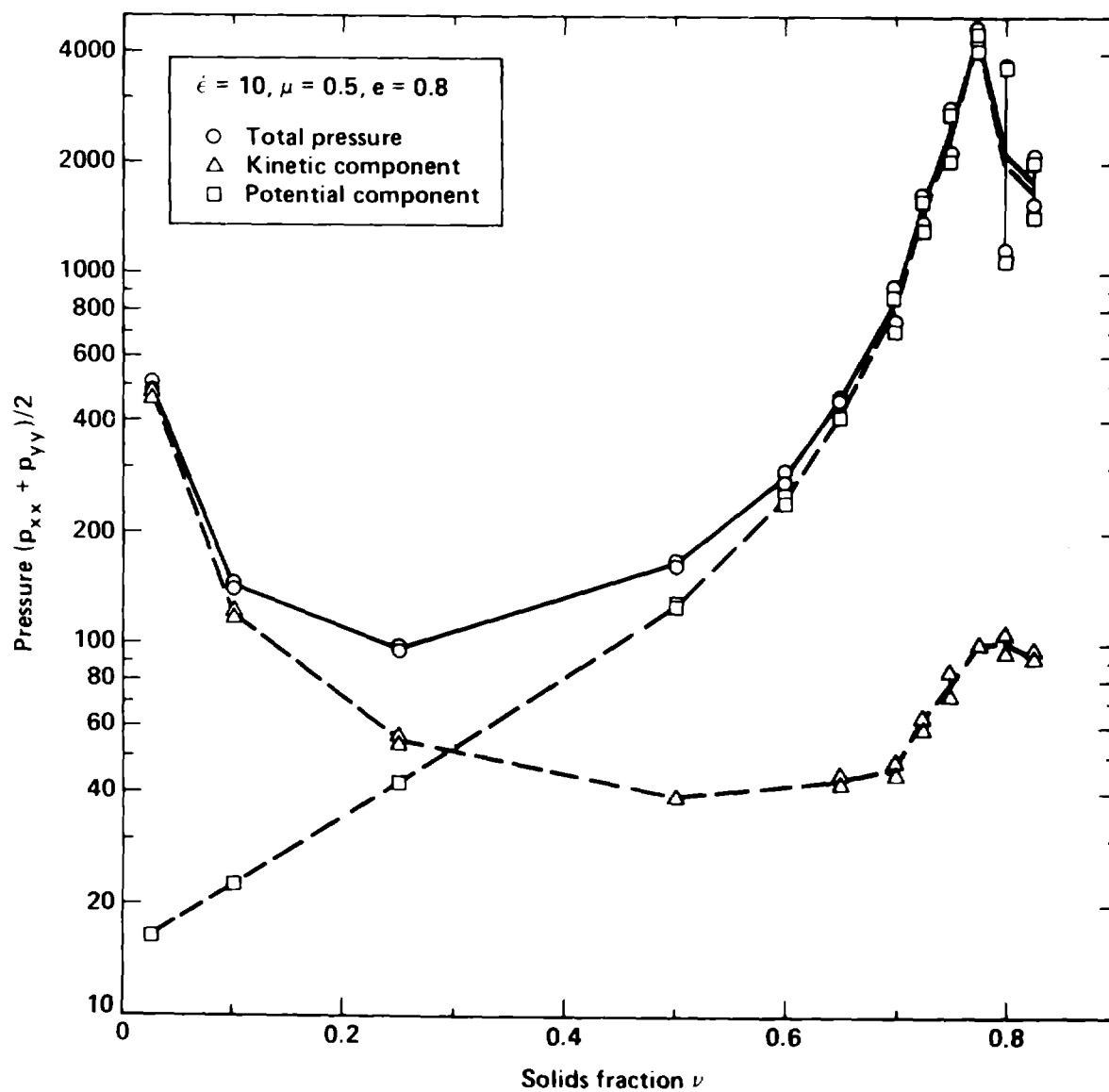


Fig. 3. Calculated total pressure, kinetic, and collisional components of the pressure for 30 inelastic, frictional particles in steady shear flow. Symbols represent time average for each calculation at each condition.

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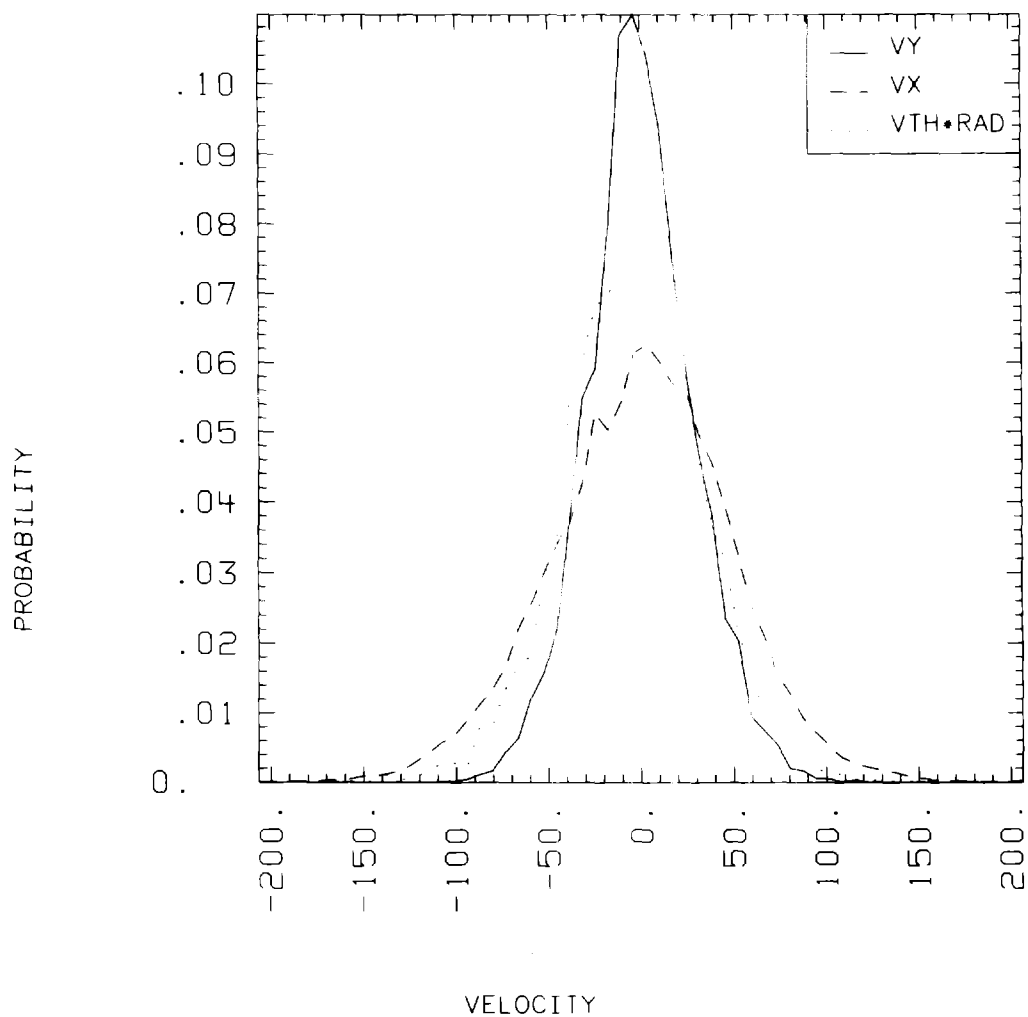


Fig. 4. cumulative time average of velocity probability distributions in the x, y, and θ directions for a set of 30 particles in steady shear with solids fraction $\nu = 0.10$, $e = 0.6$, $\mu = 0.50$.